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JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Theory of Condensed Matter: Hard Condensed Matter

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Stanislav Chadov
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Constructive Aspects of Disorder in Solids

Most of the material science problems can be reduced to a rather generic formulation: how to increase an intensity of the useful properties or how to get rid of the unwanted ones. Diversity of the degrees of freedom in complex systems makes such “signal-to-noise” control rather sophisticated and expensive. Within the state-of-the-art nano-scale applications the quality requirements for the basic technological elements are often stringent: high crystalline order, precision of target compositions, chemical or mechanical compatibility between different materials, precise number of atomic layers, etc. Once these requirements appear to be too resource-demanding, one might think about the alternatives provided by disorder. In this context, certain improvement can be achieved by introducing a specific type of disorder, suppressing the “noise” intensity, but retaining the “signal”. On the nano-scale, such engineering requires the established relationships between the properties, electronic structure, and a particular type of disorder. Here I would like to discuss the modelling of certain constructive aspects, based on the ab-initio techniques dealing with disorder explicitly (Coherent Potential Approximation and its recent extensions). In particular, I will focus on the example of the alternative half-metallicity induced by the spin-selective electron localization tuned by the chemical disorder within the class of Heusler materials.

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